

Pair Wave Functions in Atomic Fermi Condensates

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Abstract

Recent experiments have observed condensation behavior in a strongly interacting system of fermionic atoms. We interpret these observations in terms of a mean-field version of resonance superfluidity theory. We find that the objects condensed are not bosonic molecules composed of bound fermion pairs, but are rather spatially correlated Cooper pairs whose coherence length is comparable to the mean spacing between atoms. We propose experiments that will help to further probe these novel pairs.

Fermi condensates have been recently observed in dilute atomic gases, first in ^{40}K [1] and subsequently in ^6Li [2, 3]. This new state of ultracold matter represents a Fermi gas so strongly interacting that Cooper pairs become correlated in physical space as well as in momentum space, similar to the pairs in high- T_c superconductors. Such materials are believed to exist in a “crossover” regime, intermediate between weak- coupling (BCS) superconductivity and Bose- Einstein condensation (BEC) of tightly bound fermion pairs [4]. An ultracold atomic Fermi system is an ideal environment to explore the crossover regime, since the effective interactions can be tuned via a magnetic field Feshbach resonance. This possibility has led to various predictions based on a “resonance superfluidity” theory of the gas [5, 6, 7]. The BEC limit of the crossover regime was already achieved experimentally in the fall of 2003, with the creation of BEC of diatomic molecules composed of fermionic atoms [8, 9, 10].

Because of its close link to high T_c superconductivity, the crossover regime has been a topic of intense theoretical investigation, beginning from its prediction [4, 11, 12] and continuing through its recent adaptation to ultracold atomic gases [5, 6, 7, 13, 14, 15, 16]. A primary outcome of crossover theory is that the Cooper pairs begin to become localized in space due to many-body correlations as the interparticle interaction becomes large and attractive. In the high- T_c superconductor literature, these pairs are referred to as “pre-formed bosons, which can exist both above and below their transition temperature to a Bose-condensed state. The pairs in the crossover region are smaller than traditionally delocalized Cooper pairs, yet are not rigorously bound molecules. In this Letter we explore the link between pairs in the crossover regime and molecules by explicitly constructing their wave functions for the conditions of the experiment in Ref. [1]. We find that the pairs evolve smoothly into real molecules as the scattering length is tuned from negative to positive values. We also suggest experiments whereby the spatial correlations of the pairs can be probed. Note that a recent preprint comes to a similar conclusion for a uniform (i.e., untrapped) Fermi gas [17].

This finding runs counter to the expectations of Refs. [2, 13, 14], where the pairs are identified with actual molecules that are associated with the closed channel wave function in two-body scattering theory. If this were the case, then the pair wave function would decay exponentially as a function of interparticle separation, regardless of which side of the resonance it is on. That this is not the case will be demonstrated below. Additionally,

Ref. [13] identified the onset of the crossover regime by setting the binding energy of the molecule, \hbar^2/ma^2 equal to the Fermi energy $\hbar^2(3\pi^2n)^{2/3}/2m$, where m is the atomic mass and n is the number density of atoms. Doing so, one finds that in this regime the scattering length (hence the molecular size) is comparable to the interatomic spacing, and the pairs are not yet recognizable as distinct molecules. They should rather be considered as spatially correlated objects.

Accordingly, we study in this Letter the correlation length of atom pairs. Our starting point is the resonance superfluidity approach [18] adapted within the Thomas-Fermi description [19]. For concreteness, we consider the two- component Fermi gas of ^{40}K near a Feshbach resonance between the $|9/2 - 9/2\rangle$ and $|9/2 - 7/2\rangle$ states [20]. This system possesses a Feshbach resonance whose zero-energy scattering is described by an s-wave scattering length parametrized by $a(B) = a_{bg}(1 - w/\Delta B)$, with $a_{bg} = 174a_0$, $w = 7.8$ G, and ΔB is the magnetic field detuning in Gauss. For our numerical simulation we have chosen the radial frequency $\nu_r = 400\text{Hz}$ and the trap aspect ratio $\nu_r/\nu_z = 80$, as in Ref. [1].

The primary objects of the resonance superfluidity theory are the normal and anomalous densities, ρ and κ , representing the density of atoms in each species and of correlated pairs, respectively. κ can be regarded as the wave function of pairs. Because we work in the local density approximation, it is convenient to define these quantities as functions of the location \mathbf{R} of each pair's center-of-mass in the trap, and the relative momentum \mathbf{k} of the pair. The equations of motion for these quantities take the BCS-type form [6, 7, 19]:

$$\begin{aligned}
\rho(\mathbf{k}, \mathbf{R}) &= n(\mathbf{k}, \mathbf{R})u^2(\mathbf{k}, \mathbf{R}) + (1 - n(\mathbf{k}, \mathbf{R}))v^2(\mathbf{k}, \mathbf{R}), \\
\kappa(\mathbf{k}, \mathbf{R}) &= u(\mathbf{k}, \mathbf{R})v(\mathbf{k}, \mathbf{R})(1 - 2n(\mathbf{k}, \mathbf{R})) \\
E(\mathbf{k}, \mathbf{R}) &= \sqrt{h(\mathbf{k}, \mathbf{R})^2 + \Delta(\mathbf{R})^2}; \quad \begin{pmatrix} u^2(\mathbf{k}, \mathbf{R}) \\ v^2(\mathbf{k}, \mathbf{R}) \end{pmatrix} = \frac{1}{2}(1 \pm \frac{h(\mathbf{k}, \mathbf{R})}{E(\mathbf{k}, \mathbf{R})}) \\
h(\mathbf{k}, \mathbf{R}) &= \frac{\hbar^2 k^2}{2m} + V_{mf}(\mathbf{R}) + V_{trap}(\mathbf{R}) - \lambda_c \quad (1) \\
V_{mf}(\mathbf{R}) &= V_{bg}\rho(\mathbf{R}); \quad \rho(\mathbf{R}) = \int \frac{d^3k}{(2\pi)^3} \rho(\mathbf{k}, \mathbf{R}) \\
\Delta(\mathbf{R}) &= -V_{bg} \int \frac{d^3k}{(2\pi)^3} \kappa(\mathbf{k}, \mathbf{R}) - g\phi(\mathbf{R}); \quad \phi(\mathbf{R}) = \frac{g}{2\lambda_c - \nu} \int \frac{d^3k}{(2\pi)^3} \kappa(\mathbf{k}, \mathbf{R})
\end{aligned}$$

where $n(\mathbf{k}, \mathbf{R}) = (\exp(E(\mathbf{k}, \mathbf{R})/k_B T) + 1)^{-1}$ is the Fermi-Dirac distribution, $V_{mf}(\mathbf{R})$ is the mean field potential, $\Delta(\mathbf{R})$ is the energy gap, $V_{bg} = 4\pi\hbar^2 a_{bg}/m$, a_{bg} is the background (non-resonant) contact interaction, $\nu = (B - B_0)\Delta\mu$ is the detuning in energy

units, $g = \sqrt{V_{bg}\Delta B\Delta\mu}$ is a coupling representing the conversion of free fermions into pairs, ΔB is the field width of the resonance, $\Delta\mu$ is the magnetic moment difference between two hyper- fine levels of the two-component Fermi gas, λ_c is the chemical potential, and V_{trap} is the external atomic harmonic trapping potential. The chemical potential is fixed by conservation of the mean number of atoms N . In this theory, a “molecular field” ϕ is introduced to simplify the theoretical description of free fermions transforming into spatially correlated pairs. Notice that ϕ is not a distinct physical entity, but is determined once κ is known.

Though derived for interacting fermions, equations [1] can also be applied in the BEC limit [4, 21, 22] In this limit it is well- known that $(v^2(\mathbf{k}, \mathbf{R}) \ll 1)$ and that the BCS equation for the gap reduces to the Schrödinger equation for the relative motion of two interacting bosons, with energy eigenvalue $2\lambda_c = \hbar^2/ma^2$ representing the binding energy of the (rigorously bound) bosonic molecules [21, 23]. After a simple derivation we can extend this result to the case of trapped atoms. Then the pair distribution function becomes, in the BEC limit,

$$\kappa(\mathbf{k}, \mathbf{R}) = \frac{m\Delta(\mathbf{R})a^2}{k^2a^2 + 1} = \frac{\sqrt{8\pi}a^3}{k^2a^2 + 1} * \Phi(\mathbf{R}), \quad (2)$$

where $\Phi(\mathbf{R}) = \sqrt{\frac{m^2a}{8\pi}}\Delta(\mathbf{R})$ as derived in [24]. This reference also demonstrated that HFB equations transform into the Gross- Pitaevskii equation and that $\Phi(\mathbf{R})$ serves as a solution for a molecular BEC interacting through a repulsive interaction with scattering length $a_B = 2a$. This result holds in the BEC limit, where $\Delta/|\lambda_c| \ll 1$. (A more careful analysis, following [25], will give corrections, but this is not the main goal of this Letter.) Moreover, the first term on the right-hand side of Eqn. (2) is the Fourier transform of the molecular wave function $\frac{1}{\sqrt{2\pi a}}\frac{e^{-r/a}}{r}$ in the relative coordinate r . In this way the same wave function κ that represents Cooper pairs on the BCS side of the resonance actually represents a condensate of real molecular bosons on the BEC side. In general this molecular wave function depends on \mathbf{R} , meaning that the gas may contain molecules in its high-density center, but correlated Fermi pairs at its lower-density periphery. For example in this case twice the chemical potential is not quite the molecular binding energy but slightly depends on density [23].

The number of pairs can be calculated from the anomalous density as $N_b = \int d\mathbf{R}d\mathbf{k}\kappa(\mathbf{k}, \mathbf{R})^2$. In the BEC limit $\kappa(\mathbf{k}, \mathbf{R})^2 \Rightarrow \rho(\mathbf{k}, \mathbf{R})$ for small temperatures, which means that almost all atoms are paired. Moreover, using (1, 2) it is easy to check that in this limit

the density of pairs transform into the density of real molecules:

$$\rho_b(\mathbf{R}) = \int d\mathbf{k} \kappa(\mathbf{k}, \mathbf{R})^2 = \Phi(\mathbf{R})^2 \quad (3)$$

Thus the same function $\kappa(\mathbf{k}, \mathbf{R})$ describes the density of Cooper pairs away from resonance, pairs in the crossover regime, and molecules on the BEC side of the resonance as the detuning is varied.

The many-body physics of the crossover regime can be quantified in terms of a 'smooth' parameter such as the pair coherence length, usually defined as the rms radius of the pair [21]:

$$\xi^2(\mathbf{R}) = \int d\mathbf{r} \kappa(\mathbf{r}, \mathbf{R})^2 r^2 / \int d\mathbf{r} \kappa(\mathbf{r}, \mathbf{R})^2 \approx (k_F(\mathbf{R})/m\pi\Delta(\mathbf{R}))^2 \quad (4)$$

Using the above result, it is clear that in the BEC limit $\langle r^2 \rangle = a^2/2$ in the center of the trap (note that the size of a molecule is usually taken instead as the mean value of r , $\langle r \rangle = a/2$). On the BCS side of the resonance $\sqrt{\xi^2(\mathbf{R})}$ defines the 'size' of the Cooper pair. Thus the calculation of the coherence length gives us an insight of how the pairs evolve in the crossover regime.

We present the coherence length versus detuning in Fig. 1 (solid line) for the trap aspect ratio, number of atoms, and temperature of the JILA experiment [1]. For detunings $\Delta B > 0.5$ G the coherence length approaches the familiar BCS result (dash-dot line). For negative detunings $\Delta B < -1$ G on the BEC side of the resonance, the molecular size approaches the size evaluated from two-body theory (dashed line). In between, the coherence length varies smoothly, illustrating the gradual evolution of pairs into molecules. The sizes of these objects remain finite across the resonance, in spite of the divergent behavior of the scattering length. This size suppression is the result of many-body physics in the unitarity limit of $k_F a > 1$, where the physics of the gas is expected to saturate and to depend only weakly on the scattering length.

To illustrate in greater detail the smoothness of the transition between pairs in the crossover regime and molecules, we consider their wave functions, as shown in Fig. 2. This figure shows pair wave functions $r \cdot \kappa(\mathbf{r}, \mathbf{R} = 0)$ in the center of the trap, for detunings corresponding to "ordinary" Cooper pairs ($\Delta B = 1.0$ G, a), pairs in the crossover regime ($\Delta B = 0.1$ G, b), and molecules ($\Delta B = -0.5$ G, c). Wave functions of the pairs decay away on a length scale set by the coherence length, but in an oscillatory way reminiscent of a damped harmonic oscillator. This behavior is a many-body effect, and in fact the scale of the oscillation is set by the interparticle distance (solid bar). The relative motion of true molecular

bound states of course decay strictly exponentially, as in Fig.2c). For small detuning, however, the correlation length becomes comparable to the molecular size, and the ringing wave functions begin to resemble overdamped oscillators, i.e., they decay exponentially (Fig.2b). In this way the character of the pair wave functions evolve smoothly into molecular wave functions. This interpretation is somewhat complicated by the fact that the shape of pair wave function strongly depends on the trap geometry. Even for small detunings but far from the trap's center the coherence length is still large.

In order to qualitatively understand the JILA experiment [1] we now consider the positive detuning, BCS side of Fig. 1. We see that at a detuning of around $0.5G$ the size of the pairs becomes comparable to the interparticle distance (dotted line in Fig. 1). This criterion marks the crossover regime, where the atom pairs are not momentum-correlated objects like BCS Cooper pairs, nor are they yet full-fledged molecules. Significantly, this detuning is approximately where a condensate fraction can be observed in the JILA experiment [1], implying that the condensed objects consist of correlated pairs rather than real molecules. To estimate the condensate fraction, we assume for simplicity that all pairs are Bose condensed at experimental temperatures, so that the condensate fraction is simply $N_b/(N/2)$. The true condensate fraction presumably depends on the (unknown) interaction between the pairs. This *in situ* condensate fraction is presented as a function of magnetic field detuning in Fig. (3) (solid line). This fraction becomes significant only for detunings less than about 0.5 Gauss from resonance, just where the size of the pairs becomes comparable to the interparticle spacing (compare Fig.1). The condensate fraction is quite large near zero detuning. In the ideal case of a uniform gas this fraction would be 1 on resonance, but it is generally smaller for a trapped gas.

In the JILA experiment, the Fermi condensate is not directly imaged, but rather is probed by a magnetic field sweep that converts the atoms into molecules. This sweep is fast enough that it does not affect the many-body properties of the gas, but slow enough that atoms are efficiently gathered into molecules. The final detuning is far below resonance ($\sim -10G$ in Ref.[1]), so that the molecules are far smaller than the pairs that are being probed. An infinitely fast sweep that instantaneously projects pairs onto molecules would therefore not yield a significant number of molecules. The condensate fraction, however, could still be a significant fraction of unity [17].

In the present calculation, we do not treat the time dependence of the magnetic field,

and therefore cannot model the experiment as performed. We can, however, suggest another experiment that could probe the crossover regime more fully. Let us consider a hypothetical experiment where it would be possible to apply an infinitely fast sweep from a positive detuning ΔB_{BCS} to a final detuning ΔB_{BEC} , i.e., literally projecting pairs onto molecules. The final condensation fraction f observed by expansion and imaging will then be defined as a product of two probabilities: the first is the projection of the pair wave function $\kappa(\mathbf{r}, \mathbf{R})$ onto the molecular wave function (2), normalized by N_b ; the second is the fraction of atoms that are paired, $(N_b/(N/2))$:

$$f(\Delta B_{BEC}, \Delta B_{BCS}) = \left(\int d\mathbf{r} d\mathbf{R} \kappa(\mathbf{r}, \mathbf{R}) \frac{1}{\sqrt{2\pi a}} \frac{e^{-r/a}}{r} \Phi(\mathbf{R}) \right)^2 * \frac{N_b}{N/2}. \quad (5)$$

This projection depends not only on the mapping of the wave function of a pair onto the wave function of the molecule but also on the condensate wave function as $\Phi(\mathbf{R})$. The fermionic condensate wave function $\kappa(\mathbf{r}, \mathbf{R})$ cannot be so easily separated as the product of center-of-mass and relative functions as in the BEC case (2). It should be said that even in BEC case the molecular wave functions in (2) will depend on \mathbf{R} , which means that the molecular size will be different from point to point in the trap. But this dependence is quite weak especially for large negative detunings, and is therefore neglected. In the case of a large positive detuning ΔB_{BCS} the size of a Cooper pair is considerably larger than the size of a molecule and the number of pairs N_b is quite small itself so the overlap integral (5) will be quite small. It is clear that the observed condensate fraction will depend on the geometry of the trap as well as on the detuning ΔB_{BEC} of the final point of the sweeping.

We have calculated the condensate fraction, as seen by this projection technique, for three different target molecules defined by ΔB_{BEC} , corresponding to molecules of sizes $a/2 = 1000a_0, 500a_0$ and $100a_0$ (Fig. 3). As anticipated, the condensate fraction measured in this way would be smaller if the pairs are projected onto smaller molecules. Thus there are two conditions required to support a large observed condensate fraction: first the ΔB_{BCS} detuning on the BCS side of the resonance should be small enough to support a considerable number of pairs compared to the total number of atoms; and second the ΔB_{BEC} on the BEC side of the resonance should be chosen so that the corresponding scattering length will not be very different from the coherence length corresponding ΔB_{BCS} . The second condition means that the size of the pair should be comparable with the size of the molecule. For the experiment with ^{40}K atoms these conditions are fulfilled for $\Delta B_{BCS} < 0.6G$ and

$\Delta B_{BEC} > -1G$. Of course these results strongly depend on the geometry of the trap and the temperature. An experimental map of $f(\Delta B_{BEC}, \Delta B_{BCS})$ should prove quite illuminating as a probe of the length scales and condensation fractions in the crossover regime.

In conclusion, we found that the recent experiment [1] can be explained semi-quantitatively by counting the number of Cooper pairs on the BCS side of the Feshbach resonance. We suggested a new scenario to probe the crossover regime by mapping the condensate of fermionic pairs on the BCS side of the resonance onto molecules on the BEC side. We found that a considerable condensate fraction can be observed when the coherence length of the pairs is on the order of the interparticle distance.

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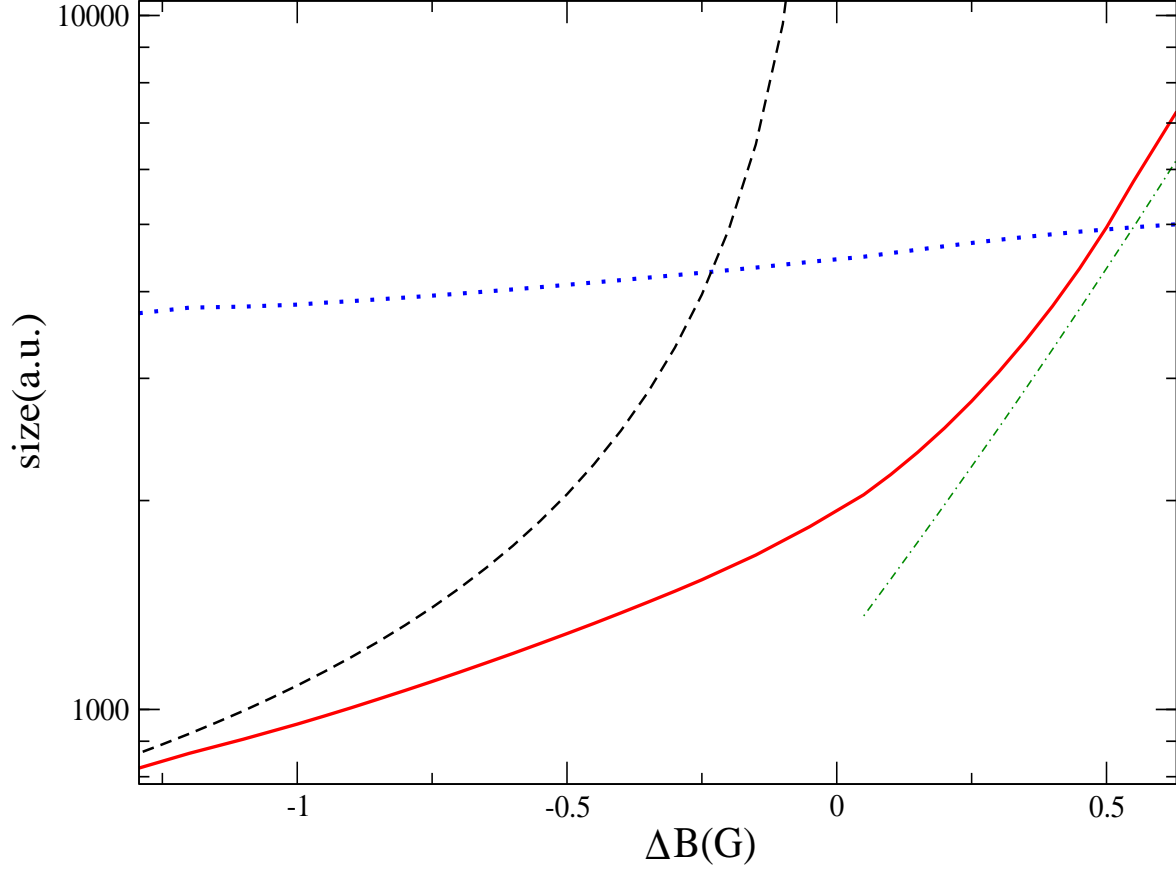


FIG. 1: Coherence length versus magnetic field detuning (solid line) for ^{40}K atoms in the JILA experiment, in the center of the trap. For comparison, the dashed curve represents the rms molecule size $a/\sqrt{2}$ corresponding to atoms with a scattering length $a = a_{bg} - \frac{g^2}{\nu}$. The dash-dotted curve is the BCS limit of the coherence length. The dotted curve represents the interparticle distance in the center of the trap. The trap aspect ratio $1/\lambda = 80$, the temperature is $T = 0.08T_F$, and the trap contains $N = 5 \times 10^5$ atoms.

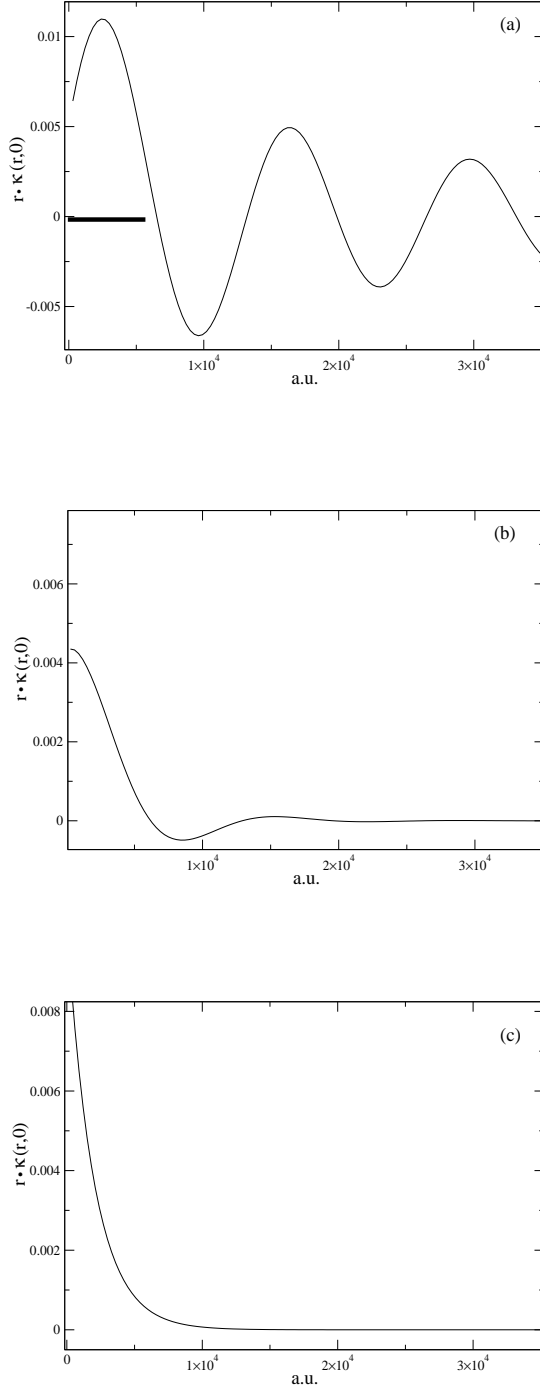


FIG. 2: Two-body correlation function $r \cdot \kappa(\mathbf{r}, \mathbf{R} = 0)$ versus interparticle separation r in the center of the trap considered in Fig. 1. The panels correspond to the detunings $\Delta B = 1.0$ G (a), $\Delta B = 0.1$ G (b), and $\Delta B = -0.5$ G (c). On the negative detuning side of the resonance, the pairs are true molecules. For comparison, the solid bar in (a) shows the interparticle distance in the center of the trap.

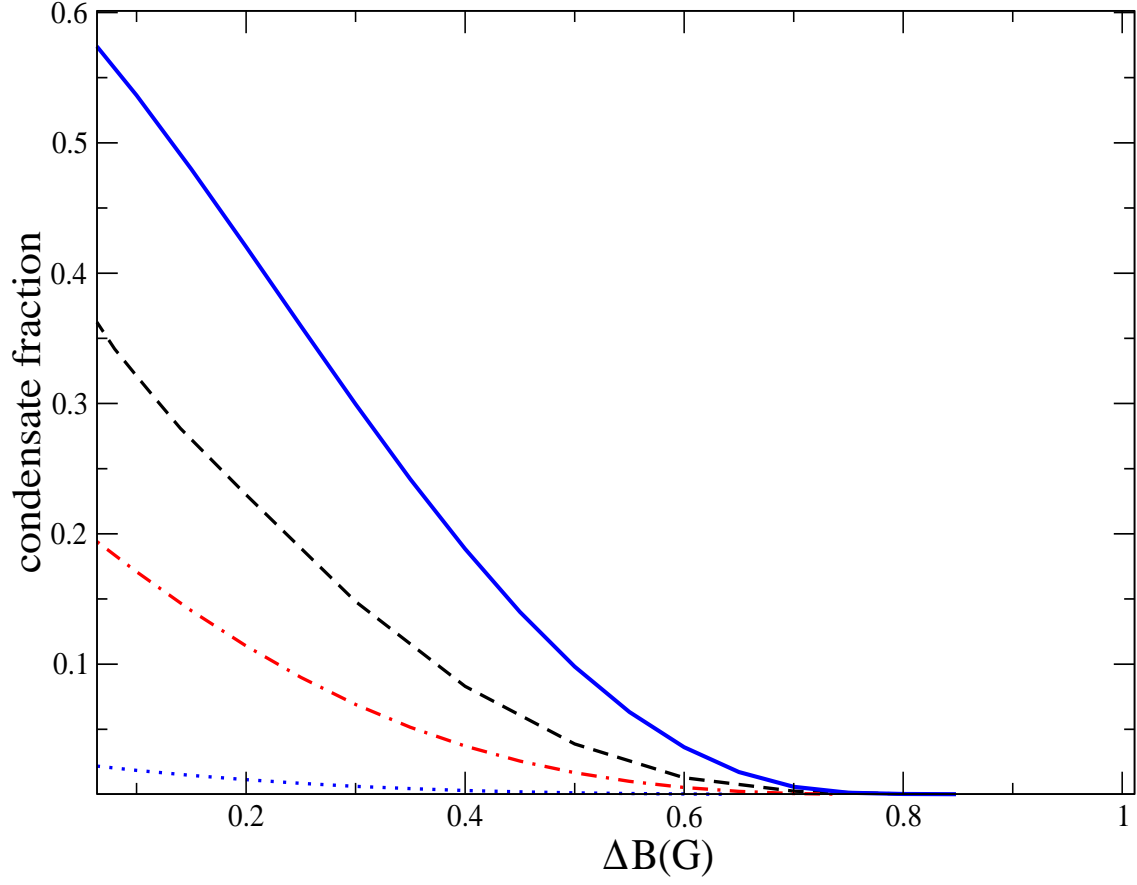


FIG. 3: Condensate fraction versus detuning, as measured by projecting onto molecules, according to Eqn. (5), for the trap considered in Fig. 1. The molecules projected onto correspond to atomic interactions with scattering lengths 2000, 1000, and 200 a_0 (dashed, dot-dashed and dotted lines respectively). The solid line is the *in situ* condensate fraction, given by $N_b/(N/2)$.